

Applicant : Skolnick et al.
Serial No. : 09/493,022
Filed : January 27, 2000
Page : 2

Attorney's Docket No.: 10886-045001 / TSRJ 655.1/
SCR 2232P

AMENDMENT

Please amend the above-captioned application as follows:

In The Claims:

Please add the following new claims:

Sub B1
A1

14. (NEW) A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

- (a) generating input data for the computer comprising:
 - (i) inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence; and
 - (ii) by way of executable code, directing the processor to produce from the alignment a three dimensional reduced protein model comprising representations of side chains of amino acid residues comprising a target protein, wherein said representations of side chains of amino acid residues are converted to interaction centers; and
- (b) outputting the three-dimensional reduced protein model to an output device or a storage area.

15. (NEW) The method of claim 14, wherein at least one interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds.

16. (NEW) A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

- (a) generating input data for the computer comprising:
 - (i) inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence; and
 - (ii) by way of executable code, directing the processor to produce from the alignment a three dimensional reduced protein model comprising representations of side chains

Applicant : Skolnick et al.
Serial N . : 09/493,022
Filed : January 27, 2000
Page : 3

Attorney's Docket No.: 10886-045001 / TSRI 655.1/
SCR 2232P

of amino acid residues comprising a target protein wherein said representations of side chains of amino acid residues are converted to interaction centers and each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds; and

(b) outputting the three-dimensional reduced protein model to an output device or a storage area.

17. (NEW) The method of claim 14 or claim 16, wherein the executable code comprises instructions for:

connecting said interaction centers by virtual covalent bonds, wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain.

18. (NEW) The method of claim 17 wherein the executable code further comprises projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain on interaction centers.

19. (NEW) The method of claim 18 wherein the executable code further comprises applying secondary constraints and/or tertiary constraints to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

20. (NEW) The method of claim 14 or claim 16, wherein the executable code comprises instructions for:

(a) connecting said interaction centers by virtual covalent bonds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy

Applicant : Skolnick et al.
Serial N : 09/493,022
Filed : January 27, 2000
Page : 4

Attorney's Docket No.: 10886-045001 / TSRI 655.1/
SCR 2232P

terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain; and

(b) projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain on interaction centers;

(c) applying secondary constraints or tertiary constraints, or, secondary constraints and tertiary constraints, to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

21. (NEW) The method of claim 14 or claim 16, wherein the target amino acid sequence comprises a sequence of less than all of the amino acid residues of a protein.

22. (NEW) The method of claim 14 or claim 16, wherein the target amino acid sequence comprises a sequence of all of the amino acid residues of a protein.

23. (NEW) The method of claim 14 or claim 16, wherein the interaction center comprises a pseudoatom representing a center of mass of a side chain.